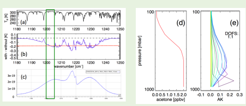
Acetone, Ethylene and Hydrogen Cyanide from Aura-TES

Susan Kulawik[1], Vivienne Payne[2], Emily Fischer[3], Dejian Fu[2]

(1) Bay Area Environmental Research Institute, Sonoma, CA, USA
(2) Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA
(3) Department of Atmospheric Science, Colorado State University, Fort Collins, Colorado, USA

Abstract We explore new chemical tracers from the Tropospheric Emission Spectrometer (Aura-TES): acetone, ethylene (C_2H_4), and hydrogen cyanide (HCN). Acetone has both biogenic and combustion sources, is a major precursor of PAN, and has an important role controlling the oxidative capacity of the upper troposphere. HCN is a unique species in that it is a combustion byproduct, dwarfing production from biogenic sources, and it can be used to trace the combustion influence of TES observations. C_2H_4 is a hydrocarbon with both biogenic and burning sources. We show the TES potential for retrieving these species, preliminary TES HCN for a major fire in Indonesia and global HCN fields for 2006. We also show spectral residuals of C_2H_4 for biomass burning land, biogenic land, burning outflow, and remote ocean locations, finding that C_2H_4 is seen in all four regions, though with considerably larger variability over sources. Acetone residuals are enhanced in both biomass burning and biogenic source regions.

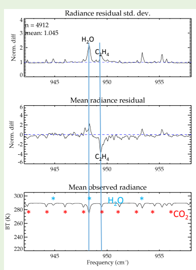
Acetone in TES spectra

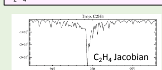


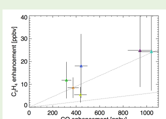
We utilize the acetone cross-section data from the HITRAN 2012 database (*Rothman et al.*, 2013; *Harrison et al.*, 2011) (a,b,c). The sensitivity is both lower and mid-Troposphere (e). The window region (1200-1205 cm^{-1}) should provide the least interference from other active species in this spectral region.

The importance of acetone . Acetone is one of the most abundant carbonyl compounds in the atmosphere. It is a precursor for peroxyacetyl nitrate (PAN) (*Fischer et al.*, 2014) and it is thought to be a major source of HO_x radicals in the upper troposphere (*McKeen et al.*, 1997; *Singh et al.*, 1995; *Wennberg et al.*, 1998). As such, acetone plays a key role in global oxidation capacity. There are major outstanding questions for acetone, and the existing observations are insufficient to answer them. Global chemical transport models do not consistently reproduce aircraft profiles or observed seasonal cycles at surface stations (e.g., *Khan et al.,* [2015]). New TES acetone measurements should provide a global, multi-year dataset with sensitivity that extends deep into the troposphere with the potential to provide new constraints on attribution in conjunction with the GEOS-Chem global chemical transport model.

C_2H_4 in TES spectra. Just prior to the C_2H_4 retrieval, the C_2H_4 feature can be seen in the radiance residual standard deviation (top) and residual mean (middle). Compare to C_2H_4 Jacobian (below, left). In the radiance (bottom), we see that this region also has CO_2 and H_2O lines. The C_2H_4 feature is about twice the size of the NESR (top, middle; as differences are divided by the NESR, 1 = size of NESR) but only about 1% the size of the radiance, and so the C_2H_4 feature does not show up by eye in the spectral plot (bottom). Although the CO2 features are larger, they are regularly spaced and well-known compared with C_2H_4.

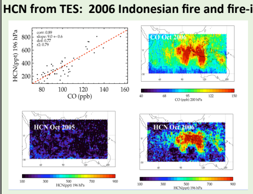




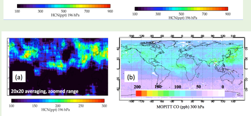


C_2H_4 seen by TES in fire plumes. C_2H_4 and CO seen in TES measurements of fire plumes during the July 2008 segment of the ARCTAS campaign show correlated enhancements (Dolan et al., 2016).

HCN from TES: 2006 Indonesian fire and fire-influence in TES observations



We utilize the HCN spectral feature at 712.5 cm^{-1} with peak sensitivity around 200 hPa. Left shows preliminary TES HCN retrievals in October 2005 (no fire, lower left) and 2006 (large fire, lower right). CO in 2006 (top right) shows a similar pattern. The upper left shows HCN (in ppt) versus CO (in ppb) for 10^{o}x10^{o} x1 month averages. The observed ratio of 9.0+/-0.6 lies within the range of tropical (4.7 ppt/ppb) and peat fires (29 ppt/ppb) quoted by *Akagi et al.* (2011). Similar HCN enhancements were seen in 2015 in this region, though with sparser coverage due to TES operations changing to special observations only.



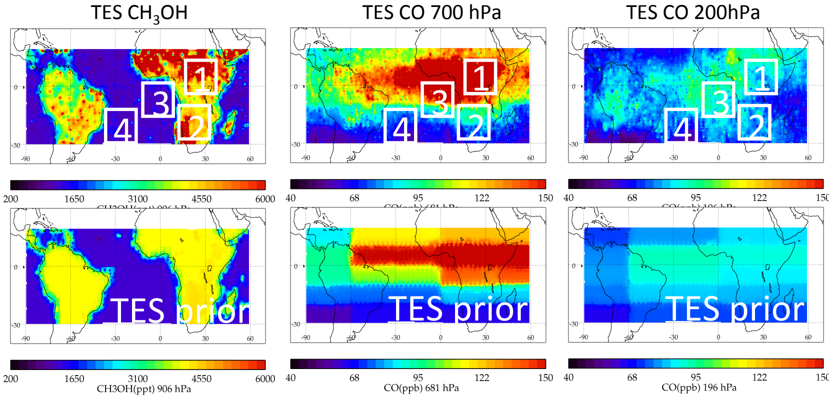
HCN as a biomass burning tracer. Above: global retrievals for June 2006 (a) alongside MOPITT CO (b). As expected, we see similar features in HCN and CO maps, due to common burning sources between these two molecules. However, CO does also have strong biogenic sources in certain regions and times of year (*Hudman et al.*, 2008).

Conclusions Spectral signatures of acetone, ethylene, and HCN are seen in TES spectra, with varying strengths in biomass burning, biogenic, outflow, and remote locations. Adding these new species to the TES products would directly address gaps in current understanding of tropospheric air quality and the oxidative capacity of the atmosphere in the following ways: (1) A better understanding of the distribution of acetone in the upper troposphere and the processes controlling it is crucial for predicting the evolution of atmospheric composition because acetone impacts oxidant distributions in this region of the atmosphere. (2) The addition of HCN and the proposed fire influence flag to the suite of existing TES retrieval products will enable new analyses of the TES data and the wider Aura and A-train measurements. (3) Previous space-based measurements of C_2H_4 have been limited either to the upper troposphere and stratosphere (limb) or to isolated fire plumes (limb and nadir). A TES C_2H_4 product is expected to provide new insight into biogenic and oceanic sources captured by C_2H_4 signals.

Support and Acknowledgements Work was performed under a contract with the National Aeronautics and Space Administration (Kevin Bowman, PI)

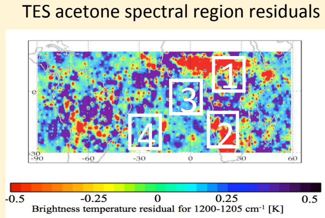
January, 2009

TES CH_3OH | TES CO 700 hPa | TES CO 200hPa



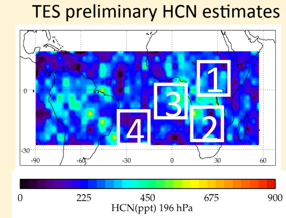
New results

TES acetone spectral region residuals



Acetone seen in biomass and biogenic regions. TES residuals in acetone region (1200-1205 cm^{-1}) show the most activity in biogenic regions (compare to TES methanol, above), with the strongest signals seen in box 1 (burning) and 2 (biogenic).

TES preliminary HCN estimates

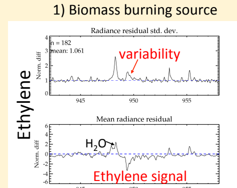


TES HCN is highest in the biomass burning outflow box (box 3), is not seen in remote ocean (box 4) and seen only in the northernmost part of the biogenic source box (box 2). HCN is not seen in the biomass burning box (box 1), as TES sensitivity to HCN is at about 200 hPa rather than at the surface (compare to box 3 versus box 1 for CO at 200 hPa).

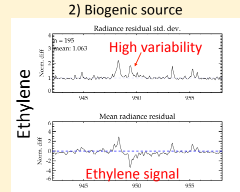
TES radiance residuals for ethylene in the following regions identified above

1) Biomass burning land (high CO): 16-36E, 5S-15N
2) Biogenic land (high CH_3OH, low CO): 12-32E, 8-28S
3) Biomass burning influenced outflow, ocean: 18S-2N,13W-7E
4) Remote ocean: 15-35W, 9-29S

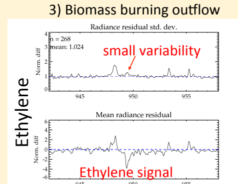
1) Biomass burning source



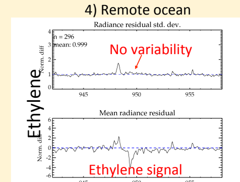
2) Biogenic source



3) Biomass burning outflow



4) Remote ocean



Ethylene residuals by region type The ethylene signal is present in all boxes, though with most variability in the biomass burning (1) and biogenic (2) source regions, little variability in the biomass burning outflow, and no variability in the remote ocean location.